Breaking a one-dimensional chain: fracture in 1 + 1 dimensions

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Abstract

The breaking rate of an atomic chain stretched at zero temperature by a constant force can be calculated in a quasiclassical approximation by finding the localized solutions ("bounces") of the equations of classical dynamics in imaginary time. We show that this theory is related to the critical cracks of stressed solids, because the world lines of the atoms in the chain form a two-dimensional crystal, and the bounce is a crack configuration in (unstable) mechanical equilibrium. Thus the tunneling time, Action, and breaking rate in the limit of small forces are determined by the classical results of Griffith. For the limit of large forces we give an exact bounce solution that describes the quantum fracture and classical crack close to the limit of mechanical stability. This limit can be viewed as a critical phenomenon for which we establish a Levanyuk-Ginzburg criterion of weakness of fluctuations, and propose a scaling argument for the critical regime. The post-tunneling dynamics is understood by the analytic continuation of the bounce solutions to real time.

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I. INTRODUCTION

A stretched solid breaks instantaneously when the external widening stress exceeds a critical value corresponding to the limit of mechanical stability of the system. For smaller stresses the fracture is time-delayed and assisted by thermal fluctuations. At sufficiently low temperatures there can be quantum effects, and the breaking rate becomes temperature independent. This last situation is the main subject of this paper.

We consider a one-dimensional system (for example, a polymer chain or nanotube) stretched by a constant external force applied at the chain ends at zero temperature, where quantum tunneling is the only mechanism responsible for the fracture. There have been several attempts in the past to study this problem [1] [2] however its many-body nature was not taken into account until the pioneering work of Dyakonov [3], who gave qualitatively correct results in the limits of weak and large external forces. A more precise analytical approach to the problem valid for small external forces has been suggested recently by Levitov *et al* [4].

We will adopt a general formalism that allows us to look at various limits from a single viewpoint. According to Feynman [5] the tunneling rate per unit length is given by $w \propto |\sum \exp(-A/\hbar)|^2$ where A is the imaginary-time Action calculated along particle trajectories connecting the "initial" (stretched) and "final" (broken) states of the chain, $\hbar$ is Planck's constant, and the summation is performed over all trajectories. In the quasiclassical limit the trajectories contributing most to the sum satisfy the stationarity condition $\delta A = 0$. These trajectories describe how the system traverses the classically- forbidden region, going from an unbroken chain into a configuration from which even a classical chain released at rest would break irreversibly. It is convenient to combine this motion with its time reversal to form a localized path called a "bounce" [6]. In the quasiclassical approximation the tunneling rate is given by

$$w \cong B \exp(-A_{bounce}/\hbar) \tag{1}$$

where the amplitude B and action A_{bounce} are calculated for the bounce (there is no factor of 2 in the exponential from the squaring because the bounce covers both the past and future). We will demonstrate below that the problem of finding bounce solutions is identical to the classical problem of finding the equilibrium crack configuration for a two-dimensional solid stretched by a constant uniaxial stress – yet another example of the correspondence between one-dimensional quantum field theory and two-dimensional statistical mechanics [7]. In view of this equivalence the results of [3] and [4] are already implied by the classical works of Griffith [8].

The present contribution to this field contains two main results. First, in the limit of a large applied force close to the limit of mechanical stability we find an exact bounce solution; simultaneously this for the first time determines the equilibrium crack configuration in the large stress classical limit. Establishing the range of applicability of this solution reveals that fluctuations inevitably come into play in the immediate vicinity of the limit of mechanical stability.

Second, we show how the bounce solutions can be used to provide insight into the real time post-tunneling dynamics.

II. GENERAL FORMALISM

The imaginary-time Action describing a one-dimensional chain stretched by an external force p applied to the chain ends has the form

$$A = \int dxdt[\frac{\rho}{2}(\dot{u}^2 + c^2 u'^2) - pu'] + \int dt[V(h) - ph] \tag{2}$$

where ρ is the linear particle density, x is the spatial coordinate (along the chain length), t is the imaginary time coordinate, $u(x,t)$ is the particle displacement field, and dots and primes stand for the imaginary time (t), and spatial (x) derivatives.

The first integral is over all positions and times except for a small region near $x = 0$, where the break will appear. This separates the line into two pieces, so that for all t the field u is discontinuous: $u(x = +0, t) - u(x = -0, t) = h(t)$; however, we expect $h(t)$ to be small outside a well-defined time interval. We have defined $h(t)$ so that the distance between the two parts of the chain is $a + h$, where a is the equilibrium ($p = 0$) interparticle spacing in the chain. The coupling between the segments of the chain in the tear region is given by the potential of cohesive forces $V(h)$ which describes the interaction between the two ends of the broken chain for arbitrary separation – that is, it goes beyond the harmonic approximation.

The properties of the function $V(h)$ can be summarized as follows (Fig. 1). For $|h| \ll a$ it obeys Hooke's law: $V(h) = \rho c^2 h^2/2a$, so that the two parts of the chain are joined into one elastic medium. For large negative h, the cohesive potential increases without bound, $V(h \to -\infty) \to +\infty$, reflecting the impossibility of indefinite compression. For large positive h it approaches a constant, $V(h \to +\infty) = 2\gamma$, which is the work done in infinitely separating the halves of the chain; 2γ can also be called the bond energy and the factor of 2 is introduced to indicate that there is an energy γ associated with each free end of the half- infinite chain pieces. In what follows we will also need to know the properties of the cohesive force function $G(h) = dV/dh$ shown schematically on Fig. 2: for small h it grows linearly with $h, G(h) = \rho c^2 h/a$, reaching a maximal value $p_c \cong \rho c^2 \cong \gamma/a$ at $h = h_c \cong a$, while $G(h)$ decreases to zero as $h \to +\infty$. The parameter h_c can be called the critical bond lengthening, while p_c is the limit of mechanical stability of the system – indeed only for $p < p_c$ does $U(h) = V(h) - ph$(the total potential energy in the external field) have a metastable minimum at $h = h_1$(Fig.3) corresponding to the equilibrium stretched chain.

The bounce solution is shown schematically on Fig.4 using the imaginary time variable t as a second (space-like) coordinate. The particle world lines belonging to the two ends of the breaking chain deviate significantly from each other for a time interval and then come back together. The external force p applied at the chain ends is time-independent, therefore it is shown schematically by series of arrows of the same length pointing in the spatial (x) direction.

The Action (2) and the Figures can be interpreted as representing a two-dimensional "crystal" of particle world lines subject to a uniaxial stress p, and in this interpretation the bounce of Fig. 4 is a critical crack, poised between the small perturbations that can spontaneously heal and the large disruptions that lead to fracture. We note in passing that our point of view that the crack opening is nonzero everywhere is different from that of many classical approaches [9], which restrict the break to a finite region completely surrounded by an elastic medium. Our treatment contains the standard approach as a special case.

To see the connection to the classical fracture problem explicitly let us seek extremal paths for the Action (3) by varying u while keeping the boundary values $h(t)$ fixed. The condition $\delta A/\delta u = 0$ reduces to the Laplace equation

$$d^2u/dt^2 + c^2u'' = 0 \tag{3}$$

The solution to (3) satisfying the boundary conditions $u(x = \pm 0, t) = \pm h(t)/2$ has the form

$$\begin{aligned} u(x,t) = \frac{p}{\rho c^2}x + \frac{signx}{2}\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}h(\omega)\exp[i\omega t - (|\omega||x|/c)] \\ \equiv \frac{p}{\rho c^2}x + \frac{x}{2\pi c}\int_{-\infty}^{+\infty}\frac{dt'h(t')}{(t'-t)^2 + x^2/c^2} \end{aligned} \tag{4}$$

where the first term describes the stretched chain, the second is due to the break, and the Fourier transform $h(\omega) = \int h(t)\exp(-i\omega t)dt$ has been introduced. Substituting (4) in (2), integrating over x, and ignoring overall constants we find the Action in a form that depends only on the field h

$$A = -\frac{D}{2}\int_{|t-t'|\geq t_0}\dot{h}(t)dt\ln(|t-t'|/t_0)\dot{h}(t')dt' + \int dt[V(h) - ph] \tag{5}$$

where $D = \rho c/2\pi$ and $t_0 \cong a/c$ is a cutoff introduced to prevent singularities for $t \to t'$. If imaginary time is viewed as a space-like variable then the Action (5) can be interpreted as a Hamiltonian describing a "crack" in a two-dimensional "crystal" of particle world lines. The crack can be represented by a distribution of fictitious dislocations [9], and then the first term of (5) describes the logarithmic interaction of these dislocations with each other with an interaction strength D, a "dislocation density" given by $-\dot{h}$, and "Burgers vectors" pointing along the chain. Similarly the second integral in (5) can be thought of as describing the cohesive interaction $V(h)$ between the sides of the "crack" in the presence of the external opening field p. A free-energy functional similar to (5) has been proposed in [10] and [11] as a field-theoretical starting point of classical fracture mechanics.

The configuration $h(t)$ for which (5) is extremal is determined by the condition $\delta A/\delta h = 0$:

$$D\int_{-\infty}^{+\infty}\frac{\dot{h}(t')}{t'-t}dt' = G(h) - p \tag{6}$$

Here and below the singular integral is taken as a principal value. A model of cracks based on a singular nonlinear integral equation of the form (6) has been analyzed by Blekherman and Indenbom [12].

The sound velocity c sets the upper limit on the value of $|\dot{h}|$, therefore the physical solutions to (6) should satisfy $|\dot{h}(t)/c| \leq 1$; at the same time the field $h(t)$ can take on arbitrarily large values.

A bounce solution to (6) will have the following form (Figs. 3, 4). For $t \to -\infty$ the function $h(t)$ starts at the metastable minimum of the total potential $U(h), h = h_1$, then makes an excursion past the unstable maximum, $h = h_2$, and comes back to $h = h_1$ as $t \to +\infty$.

Substituting (6) into (5) and subtracting from the result the Action of the stretched unbroken chain ($h = h_1$), we find the tunneling Action that goes into the probability (1)

$$A_{bounce} = \int_{-\infty}^{+\infty} dt[U(h) - U(h_1) - \frac{h - h_1}{2}\frac{dU(h)}{dh}] \tag{7}$$

where we used the result due to Blekherman and Indenbom [12] that $\int_{-\infty}^{+\infty} dt[G(h) - p] = 0$ (total zero force along the tear) for the solution to (6) satisfying $h(\pm\infty) = h_1$.

For large $|t|$ we can use a harmonic approximation, since the function $h(t)$ is close to its asymptotic limit h_1. Thus we introduce $\varphi = h - h_1$ and approximate the right-hand side of (6) by $U''(h_1)\varphi$, valid for $|\varphi| \ll a$. Expanding the integrand of (6) in t'/t and noting that $h(t)$ is even in t we find

$$\varphi(t \to \pm\infty) = \frac{D}{t^2 U''(h_1)} \int_{-\infty}^{+\infty} \varphi(t')dt' \tag{8}$$

However, this is not very interesting, since within the harmonic approximation the tunneling Action (7) vanishes.

Further progress can be made by looking separately at the cases of weak and strong tearing force where the tunneling Action can be computed in a controlled fashion.

III. SMALL-FORCE LIMIT, P$\ll$ P$_C$

In studying the weak force limit, $p \ll p_c$, we can import some ideas from classical fracture mechanics**.** The position of the unstable maximum ($h = h_2$) of the function $U(h)$ (Fig.3) shifts to infinity as $p \to 0$. However the amplitude of the bounce solution must be larger than h_2, thus implying that over some time the distance between the edges of the tear is much bigger than equilibrium interparticle spacing. Since the bounce tail (8) does not contribute to the tunneling Action (7) in quadratic order, we can take h to be nonzero only within a time interval $-L < t < L$(Fig.4). The tunneling time 2L will be determined later. The cohesive force, $G(h)$, is negligible for $-L \le t \le L$ and operative beyond this interval. The latter feature implies that there is a strain outside the segment $[-L; L]$ that takes care of the assumed $h(t) = 0$. Then (6) simplifies to

$$D \int_{-L}^{+L} \frac{\dot{h}(t')}{t' - t} dt' = -p \tag{9}$$

for $-L \le t \le$ L. Neglect of the cohesive forces within the tunneling interval implies that the edges of the tear are force free, i.e. $u'(x = \pm 0, t) = 0$; this condition applied to the representation (4) with the limits of the integration set by $-L$ and L indeed reproduces (9).

In the same approximation the total potential $U(h) = V(h) - ph$ can be replaced by $U(h) = 2\gamma - ph$, and (7) simplifies to

$$A_{bounce} = \int_{-L}^{+L} dt(2\gamma - \frac{1}{2}ph) \tag{10}$$

where for $p \ll p_c$ we neglected $U(h_1) + ph_1/2 = -p^2 a/\rho c^2$ compared to 2γ. The solution to (9) satisfying $h(\pm L) = 0$ is the elliptical crack of fracture mechanics [13] [14]:

$$h(t) = \frac{p}{\pi D}\sqrt{L^2 - t^2} \equiv \frac{2p}{\rho c}\sqrt{L^2 - t^2} \tag{11}$$

Substituting this into (10) and evaluating the integral we find

$$A_{bounce}(L) = 4\gamma L - p^2 L^2/4D \tag{12}$$

This expression determines the Action parameterized by the time $2L$, which is chosen so that $A_{bounce}(L)$ is extremal: then the Action is stationary with respect to all variations in the path connecting broken to unbroken configurations. Eq. (12) has a maximum at

$$2L_G = 16\gamma D/p^2 \equiv 8\gamma\rho c/\pi p^2 \tag{13}$$

which is identified as the tunneling time. In the context of classical fracture mechanics this is called the Griffith criterion [8] [9]. Combining (1), (12), and (13) we find that for $p \ll p_c$ the fracture rate (per unit time and per unit length of the chain) is given by

$$\begin{aligned} w &\cong (1/cL_G^2)\exp[-A_{bounce}(L_G)/\hbar] \cong (p^4/\gamma^2 D^2 c)\exp(-16\gamma^2 D/\hbar p^2) \\ &\cong (p^4/\gamma^2\rho^2 c^3)\exp(-8\gamma^2\rho c/\pi\hbar p^2) \end{aligned} \tag{14}$$

where the prefactor B from (1) has been estimated by arguing that the break can occur anywhere in two-dimensional space-imaginary time: the prefactor $1/cL_G^2$ is the density of *independent* bounces that can fill up two-dimensional space- imaginary time (to be independent, two bounces must be separated in time by more than L_G and in space by more than cL_G).

The effective mass involved in the tunneling can be estimated from an argument parallel to that of Dyakonov [3]. The representation (4) implies that the effect of an inhomogeneity of size L_G in the t-direction perturbs the picture of the world lines over a distance of order cL_G(in the x- direction) containing about cL_G/a atoms. Each of them has a mass $m = \rho a$, therefore the effective mass M involved in the tunneling is found to be

$$M \cong m(cL_G/a) \cong m(\rho c^2\gamma/ap^2) \cong m(p_c/p)^2 \tag{15}$$

The tunneling time $2L_G$ (13), the maximal width of the tear [see Eq(11)], $h(0) = (p/\pi D)L_G = 8\gamma/\pi p$, and the tunneling mass (15) all diverge as $p \to 0$ implying that fracture through tunneling has many-body nature.

Here as in fracture mechanics this approach breaks down in the vicinity of $t = \pm L$ where the derivative $\dot{h}(t)$ diverges. There is also an associated stress singularity (which we will not discuss here) near $t = \pm L$. These defects can be remedied by taking proper account of the cohesive forces [9] [14] with the general conclusion that all the scaling dependencies predicted in the framework of the Griffith approximation are correct and that the numerical factors entering Eqs.(12)- (14) are accurate in the limit $p \ll p_c$; these comments apply equally well to the quantum fracture problem.

For example, the range of applicability of Eq(11) can be found by requiring that both $|\dot{h}| \leq c$ and $h \gg a$ with the conclusion that *independently of the value of the tearing force* p, (11) can be trusted outside a small region – a dozen microscopic time spans of order a/c in the vicinity of $t = \pm L_G$.

For $p \ll p_c$ the tail of the true solution (8) becomes

$$\varphi(t \to \pm\infty) = \frac{apL_G^2}{\rho c^2 t^2} \cong a(p/p_c)(L_G/t)^2 \tag{16}$$

which is generally small since $p \ll p_c$.

The analysis given above shows that for weak breaking forces ($p \ll p_c$) the true bounce solution is approximated quite well by Eq(11) for $|t| < L$, and by Eq.(16) for $|t| > L$, outside of the vicinity of $|t| = L = L_G$. The determination of the size of the transient region (expected to be a dozen microscopic time scales a/c) and the precise functional form $h(t)$ inside it require a detailed knowledge of the cohesive potential $V(h)$; it should not affect the main conclusions (13)-(15).

Apart from numerical and preexponential factors, the results (13) and (14) were first found by Dyakonov [3] using heuristic arguments based on the tunneling properties of a particle of effective mass (15) passing through a triangular potential barrier. A conformal mapping technique similar to what is employed in fracture mechanics [14] was used by Levitov *et al* [4]; this reproduced Eq(11) and (12), the numerical factors entering in Eq.(13) and the exponential of Eq.(14). However, the link to classical fracture mechanics has not been previously noticed.

Experimental verification of the weak tension results will be hindered by the exponentially large lifetime of the chain [see Eq.(14)]. Therefore the case of large tearing force (p close to p_c), where the lifetime is shorter, seems more important from the practical standpoint.

IV. VICINITY OF THE LIMIT OF MECHANICAL STABILITY, $\Delta P \ll P_C$

For $\Delta p = p_c - p \ll p_c$ the tunneling still has a collective nature, because the limit of mechanical stability, $p = p_c$, is formally similar to the spinodal of magnetic systems [10] [11]. In this limit the tunneling involves the vicinity of $h = h_c$(Fig.2) and the bounce amplitude is very small. Regardless of the underlying interactions the cohesive force can be approximated here as $G(h) = p_c - b(h-h_c)^2$ where $b = -\frac{1}{2}d^3V(h = h_c)/dh^3$. The zeros of $G(h) - p = \Delta p - b(h-h_c)^2$ determine the positions of the metastable minimum (h_1) and unstable maximum (h_2) of the total potential energy function $U(h)$ (see Fig. 3):

$$h_{1,2} = h_c \mp \sqrt{\Delta p/b} \tag{17}$$

Expressing $G(h) - p$ in terms of $\varphi = h - h_1$ we find

$$G(h) - p = 2\sqrt{\Delta p b}\varphi - b\varphi^2 \tag{18}$$

Similarly the potential energy function $U(h) = V(h) - ph$ can be written as

$$U(h) = U(h_1) + \sqrt{\Delta p b}\varphi^2 - \frac{b}{3}\varphi^3 \tag{19}$$

and Eqs. (6) and (18) give the equation for the bounce:

$$D\int_{-\infty}^{+\infty} \frac{\dot{\varphi}(t')dt'}{t'-t} = 2\sqrt{\Delta p b}\varphi - b\varphi^2 \tag{20}$$

Close to the limit of mechanical stability the properties of strongly stretched unbroken chain substantially deviate from those of the equilibrium one: the linear mass density ρ is significantly reduced, and the lattice looses its stiffness at $p = p_c$. The latter means that both the sound velocity c, and the parameter $D = \rho c/2\pi$ entering (20) *vanish* as $\Delta p \to 0$. The functional dependencies can be recovered by comparing the harmonic terms of (19) and (2), $\sqrt{\Delta p b} \cong \rho c^2/a$, which gives us

$$D \cong (m^2 b\Delta p)^{1/4}, c \cong a(b\Delta p/m^2)^{1/4} \tag{21}$$

The solution to Eq.(20) is

$$\varphi(t) = \Phi\frac{\xi^2}{t^2+\xi^2}, \tag{22}$$

where

$$\Phi = 4\sqrt{\Delta p/b} \tag{23}$$

$$\xi = \frac{D\pi}{2\sqrt{\Delta p b}} \cong (m^2/b\Delta p)^{1/4} \tag{24}$$

Combining (19) and (22)-(24) we see that the general "sum rule" (8) is indeed satisfied. The value of the bounce amplitude $\varphi(t=0) = \Phi$ is small close to $p = p_c$; at the same time $h(0) = \Phi + h_1 = h_c + 3\sqrt{\Delta p/b} = h_2 + 2\sqrt{\Delta p/b} > h_2$, i.e. as expected for the bounce solution, the function $h(t)$ goes past h_2 for some time.

The divergent time scale ξ (24) can be interpreted as a tunneling time, and the effective tunneling mass M can be estimated by replacing L_G by ξ in (15): $M \cong m(c\xi/a) \cong$ m. We see that as $\Delta p \to 0$ the effective mass involved in tunneling is comparable to the single particle mass in agreement with Dyakonov [3].

Substituting the potential energy function (19) into (7) with the bounce solution given by (22)-(24), and computing the integral we find for the tunneling Action

$$A_{bounce} = 2\pi^2 D\Delta p/b \cong (m^2/b^3)^{1/4}(\Delta p)^{5/4} \tag{25}$$

which in view of (1) implies that for $\Delta p \ll p_c$ the tunneling rate is given by

$$w \cong (1/c\xi^2)\exp(-2\pi^2 D\Delta p/b\hbar) \cong (b\Delta p/m^2 a^4)^{1/4}\exp[-const(m^2/b^3)^{1/4}(\Delta p)^{5/4}/\hbar] \tag{26}$$

where the prefactor is taken from (14), L_G is replaced by ξ [Eq(24)], and the dimensionless constant under the exponential is of order unity.

Our results (25) and (26) in the limit $\Delta p \ll p_c$ reproduce those of Dyakonov [3] even though he could not find the exact bounce solution (22)-(24). Even in the absence of the exact solution it can be seen that Eq(20) has a solution of the form $\varphi(t) = 4\sqrt{\Delta p/b}f(t/\xi)$ where ξ is given by (24) and f(z) is a scaling function obeying an integral equation that has no free parameters at all. This identifies $\xi \propto (\Delta p)^{-1/4}$ with the tunneling time, and then the tunneling Action is estimated as proportional to $(\Delta p)^{3/2}(\Delta p)^{-1/4} = (\Delta p)^{5/4}$ in agreement with the calculation that led to (25).

In view of the equivalence between the bounce solutions and equilibrium cracks of the corresponding two-dimensional classical problem, Eqs. (22)-(24) also give the equilibrium crack configuration in the limit of large stresses close to the limit of mechanical stability p_c. In this correspondence the imaginary time t becomes a spatial coordinate along the crack, D is an elastic constant [9] [still vanishing according to (21)], ξ is the effective length of the crack, and the parameter m will have a meaning of a typical binding energy divided by interparticle spacing. The rate of the crack nucleation will be given by (26) with the physical temperature T substituting for the Planck's constant $\hbar$.

The classical problem of finding the equilibrium crack configuration in the large stress limit close to the stability threshold was previously considered in [11]. The conclusions of that work differ from ours for two reasons. First, it was assumed that the long-range nature of the interaction between the different parts of the crack profile through the bulk of crystal can be replaced by a finite-range interaction; as a result the equation for the profile is differential rather than integral [see (20)]. However, this is certainly not true for materials obeying conventional elasticity theory. Second, it was assumed that for small φ, $G(h) - p = \Delta p - b\varphi^2$, instead of our Eq(18). But this cannot be correct, because for $\varphi = 0$(metastable equilibrium) the cohesive force $G(h)$ balances the external force p and therefore $G(h) - p$ must vanish.

V. LEVANYUK-GINZBURG CRITERION AND CRITICAL REGION

According to (25) the tunneling Action vanishes upon approach to the limit of mechanical stability $p = p_c$. However, the results of the previous Sections were based on a quasiclassical picture which is only valid for $A_{bounce}/\hbar \gg 1$, i.e. when the exponential factor of (1) dominates the breaking rate. This condition imposes a range of validity for our results

$$\Delta p/p_c \gg (b^3\hbar^4/m^2p_c^5)^{1/5} \tag{27}$$

that eliminates from consideration the immediate vicinity of the threshold of mechanical stability $p = p_c$. This condition is analogous to the Levanyuk-Ginzburg criterion [15] of weakness for thermal fluctuations in the theory of critical phenomena.

The results (21)-(26) were also obtained under the assumption that $\Delta p/p_c \ll 1$[only then is the expansion in powers of φ used in (18) - (20) accurate]. This will be consistent with (27) only if

$$\mathbf{Gi} \equiv (b^3\hbar^4/m^2p_c^5)^{1/5} \ll 1 \tag{28}$$

The dimensionless quantity **Gi** is a property of a given substance and is analogous to the Ginzburg parameter of the theory of critical phenomena. In the present context the requirement **Gi** $\ll 1$ can be viewed as the condition of weakness of quantum fluctuations.

The inequalities (27) and (28) set the range of applicability of the theory of Section IV. The immediate vicinity of $p = p_c$ corresponding to the reversed sign in the inequality (27) can be called the fluctuational region; quantum fluctuations play here a dominant role and the quasiclassical approximation is insufficient. In the case of the reversed sign in the inequality (28), **Gi** $\gg 1$, the theory of Section IV has no range of applicability at all.

For the case that one of the conditions (27), (28) is broken, our analytic approach fails, but some understanding can be gained with the aid of a scaling theory constructed in analogy with the theory of critical phenomena [16]. Assume that in the critical regime there is a single independent divergent time scale ξ, the tunneling time, and all other physical quantities can be expressed in terms of ξ. According to (19), the barrier for tunneling can be estimated as $(\Delta p)^{3/2}/b^{1/2}$, and therefore the tunneling Action behaves as $\xi(\Delta p)^{3/2}/b^{1/2}$. In the critical region the tunneling Action should be of the order of Planck's constant $\hbar$, so that

$$\xi \cong \hbar b^{1/2}/(\Delta p)^{3/2} \tag{29}$$

We also expect that the tunneling mass is still of order m which implies $c \cong a/\xi$ for the critical behavior of the sound velocity. These conjectures are made plausible by two mild self-consistency checks: (i) the divergence in (29) is stronger than (24)) as expected for the critical regime; (ii) the dependencies (29) and (24) match each other on the border of the critical regime defined by (27).

The conditions (27) and (28) have the classical analogs that the results of Section IV are applicable to the classical fracture of solids whenever the following inequalities are satisfied

$$\Delta p/p_c \gg (b^3T^4/m^2p_c^5)^{1/5} \tag{30}$$

$$\mathbf{Gi} \equiv (b^3T^4/m^2p_c^5)^{1/5} \ll 1 \tag{31}$$

Now the constraints (30) and (31) describe the conditions for thermal fluctuations to be sufficiently weak so that the critical crack described by (22)-(24) is relevant for the case of large applied stresses.

Inside the critical region, $\Delta p/p_c \ll (b^3T^4/m^2p_c^5)^{1/5}$, thermal fluctuations play a dominant role and the mean-field-like treatment of Section IV is invalid. If the Ginzburg parameter (31) is not small compared to unity, the theory of Section IV does not apply.

In the critical regime the analog of (29),

$$\xi \cong Tb^{1/2}/(\Delta p)^{3/2}, \tag{32}$$

gives the dependence of the critical crack length ξ on the distance to the instability threshold Δp.

VI. REAL TIME DYNAMICS

Coleman [6] notes that the analytic continuation of the bounce to real time describes the evolution of the system *after* the tunneling takes place. Introducing the physical time $\tau =$ -it into (11) we find that for a small tearing force, $p \ll p_c$, the separation between the pieces of the chain evolves with time as

$$h(\tau) = \frac{2p}{\rho c}\sqrt{L_G + \tau^2} \tag{33}$$

where L_G is the true tunneling time (13). Equation (33) meets our physical expectations: after penetrating through the barrier at $t = i\tau = 0$, the end of the chain starts moving

classically from rest from the escape position $h(0) = 2pL_G/\rho c = 8\gamma/\pi p$ which is the turning point of the classical motion. The result (33) is also precise analytically as in getting (11) the potential energy function $U(h)$ was approximated by $2\gamma - ph$ which is even more accurate in the classically allowed region than under the barrier.

For small times ($\tau \ll L$), $Eq.$(33) predicts a motion with a constant acceleration $2p/\rho c L_G$ that can be understood as follows. Immediately after the break each point of the chain excepting a finite segment near the edge will be in mechanical equilibrium. Therefore the whole unbalanced force p is applied to the edge segment. The mass of this region is the same as the tunneling mass (15), $M \cong \rho c L_G$, and its acceleration due to the external force p is of order $p/M \cong p/\rho c L_G$ in agreement with (33). This motion breaks the force balance of the region next to the moving edge segment causing the propagation of acceleration away from the tear.

To understand the dynamics inside the chain we use the expression [14] [4] for the displacement field $u(x,t)$ corresponding to the solution (11):

$$u(x,t) = \frac{p}{\rho c^2} Re[(x+ict)^2 + (cL_G)^2]^{1/2} \tag{34}$$

Analytically continuing this to the real time $\tau = -it$, we find

$$u(x,\tau) = \frac{p}{2\rho c^2} signx \left([(x-c\tau)^2 + (cL_G)^2]^{1/2} + [(x+c\tau)^2 + (cL_G)^2]^{1/2} \right) \tag{35}$$

This expression is a solution to the wave equation $\partial^2 u/\partial\tau^2 - c^2\partial^2 u/\partial x^2 = 0$ in the two parts of the broken chain satisfying the conditions $u(\pm 0,\tau) = \pm h(\tau)/2$ and $u'(\pm 0,\tau) = 0$. It describes sound waves propagating away from the break and leaving behind virtually unstrained material moving at constant speed. Not much is happening for $\tau < L_G$; however, for $\tau \gg L_G$ the following picture emerges (by symmetry we only need to consider the $x > 0$ segment). For $x \ll c\tau$ the strain u' is small and $u(x,\tau) \cong p\tau/\rho c$, whereas for $x \gg c\tau, \partial u/\partial\tau$ is small and $u(x,\tau) \cong px/\rho c^2 : a$ moving unstrained region encounters a stretched immobile region at $x = c\tau$. In a transition region having the width of order cL_G the matter is beginning to move to become part of the moving region. The unstrained region set into motion has mass that grows linearly with time $[M(\tau) = mc\tau/a = \rho c\tau]$ and moves at the constant speed $v = p/\rho c$; the momentum $M(\tau)v = p\tau$ is growing linearly in time in response to the constant applied force p. Figure 5 shows how this soliton-like wave traveling away from the break is presented in terms of particle trajectories. The break occurred at $x = 0$, $\tau = 0$, and the Figure was constructed by adding $u(x,\tau)$ [given by Eq.(35)] to x for each τ.

In the large force limit, $\Delta p \ll p_c$, we analytically continue the bounce solution (21) to find that the distance between the tearing edges of the chain evolves with time as

$$h(\tau) = h_1 + \Phi \frac{\xi^2}{\xi^2 - \tau^2} \tag{36}$$

Similar to the case of small tearing force, $p \ll p_c$, the initial stage of the motion, $\tau \ll \xi$,, described by Eq(36) can be interpreted as a constant acceleration of the tunneling mass m by the unbalanced force Δp. However the range of applicability of (36) is rather narrow – Eqs(22)-(24) [and thus (36)] were obtained assuming the expansions (18)) and (19) to be valid. At the same time the distance between the tearing edges grows with time according to

(36), thus implying that as time progresses, $h(\tau)-h_1$ becomes comparable to the equilibrium interparticle spacing a and the expansions (18) and (19) cease to be accurate. Therefore (36) is valid only for $\tau \ll \xi$. In the same approximation the motion in the chain can be obtained by substituting (22) in (4), evaluating the integral, and doing analytic continuation to the real time $\tau = -it$:

$$u(x,\tau) = \frac{p_c}{\rho c^2}x + \frac{signx}{2}\left(h_1 + \Phi\xi\frac{|x|/c+\xi}{[|x|/c+\xi]^2-\tau^2}\right) \tag{37}$$

where the sound velocity c is given by (21). Beyond the range $\tau \ll \xi$, the dynamics is expected to be described by a theory qualitatively similar to the one given above for the case $p \ll p_c$ with p_c and ξ substituting for p and L_G.

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REFERENCES

[1] R.L.Salganik, Dokl. Akad. Nauk SSSR **185**, 76(1969)[Sov. Phys. Dokl. **14**, 221(1969)]; Fiz. Tverd. Tela (Leningrad)**12**, 1336(1970)[Sov. Phys. Solid State **12**, 1051(1970)]; Int. J. Fracture Mech. **6**, 1, (1970).

[2] J.J.Gilman and H.C.Tong, J. Appl. Phys. **42**, 3479(1971).

[3] M.I.Dyakonov, Fiz. Tverd. Tela (Leningrad)**29**, 2587(1987)[Sov. Phys. Solid State **29**, 1493(1987)].

[4] L.S.Levitov, A.V.Shytov, and A.Yu.Yakovets, Phys. Rev. Lett. **75**, 370(1995).

[5] R.P.Feynman and A.R.Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).

[6] S.Coleman, Phys. Rev. D**15**, 2929(1977); for a full overview see papers in *Quantum Tunnelling in Condensed Media* edited by Yu.Kagan and A.J.Leggett (Elsevier, Amsterdam, 1992).

[7] J.B.Kogut, Rev. Mod. Phys.**51**, 659(1979), and references therein; a bounce is the quantum equivalent of the critical nucleus of Langer's droplet model [J.S.Langer, Ann. Phys. (N.Y.)**41**, 108(1967)].

[8] A.A.Griffith, Philos. Trans. Roy. Soc. London A**221**, 163(1920); **222**, 180(1921).

[9] L.D.Landau and E.M.Lifshitz, *Theory of Elasticity* (Pergamon, Oxford, 1986), Section 31.

[10] J.B.Rundle, J. Geophys. Res. **94**, No.B3, 2839(1989).

[11] J.B.Rundle and W.Klein, Phys. Rev. Lett. **63**, 171(1989).

[12] M.Kh.Blekherman and V.L.Indenbom, Zh. Prikl. Mekh. Tekhn. Fiz. **11**, 96(1970)[J. Appl. Mech. Tech. Phys. **11**, 94(1970)].

[13] *Theory of Elasticity* (Ref.9), Problem to Section 30.

[14] For a comprehensive review of the results and methods of classical fracture mechanics see the contributions to *Fracture*, v.II edited by H.Liebowitz (Academic Press, New York, 1968).

[15] L.D.Landau and E.M.Lifshitz, *Statistical Physics, 3rd ed.* (Pergamon, Oxford, 1980), Vol.5, Part I, Section 146.

[16] *Statistical Physics* (Ref.15), Section 149.

FIGURES

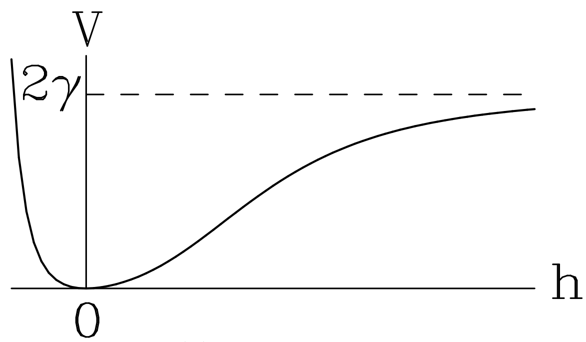

FIG. 1. The cohesive potential $V(h)$ acting between the edges of the chain segments. For $h \to \infty$ it saturates at the value 2γ corresponding to the bond energy.

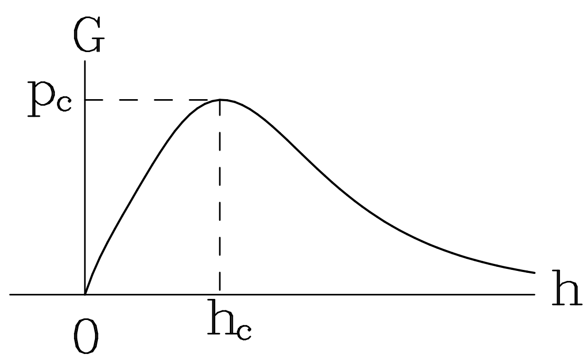

FIG. 2. The cohesive force $G(h) = dV/dh$. It reaches a maximal value p_c at the critical bond lengthening h_c which corresponds to the limit of the mechanical stability of the system.

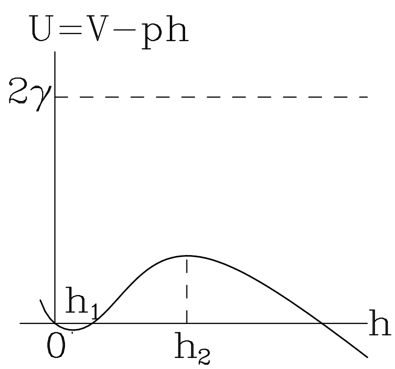

FIG. 3. The total potential energy $U(h) = V(h) - ph$. In the presence of an external tearing force $p < p_c$ the total potential energy has a metastable minimum at h_1 describing the untorn stretched chain and an unstable maximum at h_2, which is the position of the peak of the tunneling barrier.

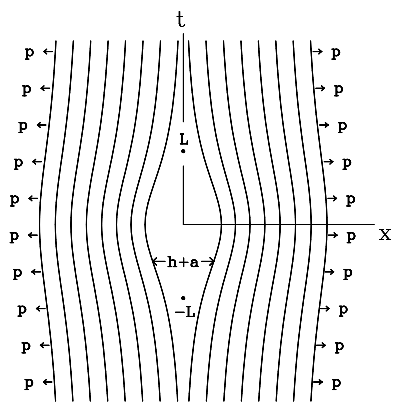

FIG. 4.   The two-dimensional "crystal" of particle world lines torn by a constant external force p traversing the imaginary time (t) direction. The tear takes place at $x = 0$, the distance between the torn edges is $h + a$, the tunneling time is 2L, and the system penetrates through the barrier at $t = 0$.

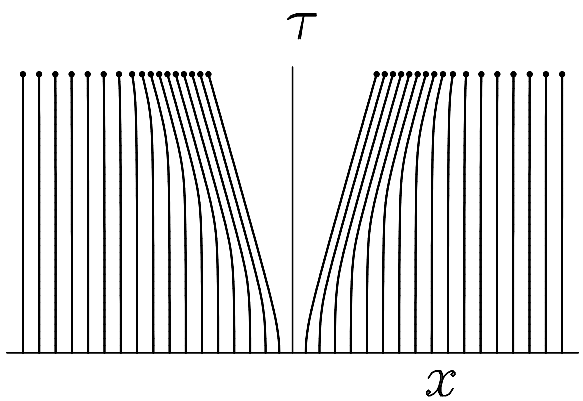

FIG. 5.   The collection of particle trajectories constituting a breaking one-dimensional solid torn by a constant external force p.